Nuclear Engineering – Group E
Whole Core/System Code - Neutronics

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Outline

- Goal
- Current methods
- New methods
- Conclusions / high end computing needs
- Coarse mesh transport method – Collaborative effort of Georgia Tech, INL and Penn State

Goal

- Develop a code system for new generation of reactors to perform highly efficient and accurate
  - whole core simulation (neutron and photon)
    - Design, optimization and online simulation
  - reactor vessel shielding calculation including a detailed model of the whole core

Goal-2

How?

- Develop a 3-D whole core (system) coupled neutron and photon transport method which
  - Is based solely on transport theory
  - Does not require cross-section homogenization
  - Contains an accurate and self-consistent global flux and dose reconstruction procedure
  - Is applicable to large complex heterogeneous reactors
  - And is ideally based on continuous energy cross sections (avoid multigroup theory)

Requirement:

- This code must
  - accommodate seamless coupling to the CFD code/module
  - be highly accurate and efficient
  - not rely on massive computers for production and online simulations

Current Methods

- Two phase approach
  - Divide reactor into homogenized coarse meshes of assembly size
  - Generate homogenized cross sections using transport theory
  - Use homogenized cross sections to perform whole core diffusion calculations
  - Thermal hydraulics is embedded as a module within the diffusion simulator (returns coolant density and temperature given the fuel pin power distribution)
- Accuracy acceptable for operating reactors
  - The simulator is tuned to reactor type/design
- Large but manageable CPU for lattice calculations (precomputation: data library generation)
  - No need for parallelization
- Whole core calculations are highly efficient (seconds)
  - Accuracy deteriorates with increasing heterogeneity
  - Data (cross section library) handling and storage are not an issue

New Methods

- Current trend is to avoid use of diffusion theory in favor of pure transport theory
- Methods under development worldwide
  - Continuous energy Monte Carlo
  - Direct fine mesh transport
  - Coarse mesh transport
    - Hybrid Monte Carlo and deterministic
    - Pure deterministic
  - Low order coarse mesh transport with and without homogenization

Direct Monte Carlo

- Advantages
  - Complex geometry
  - Highly accurate
  - No phase space discretization
  - Continuous energy cross sections treatment
- Disadvantages
  - Plagued by statistical uncertainties
  - Requires large CPU
  - Obtaining detailed (e.g., pin power distribution) solution increases CPU substantially for large (reactor) problems
  - Potential problems
    - Source convergence for systems with very short MFP
    - Deep penetration shielding calculations

Direct Fine Mesh Transport

- Current methods inefficient for whole core transport
  - Significant memory and CPU requirement
  - High order approximation is needed in heterogeneous configurations
- Requires substantial improvements/development, e.g.,
  - Acceleration techniques
  - Data handling
  - Parallel environment
  - Phase space decomposition
  - Variable meshing
  - Adaptive phase space discretization or differencing scheme and approximation order

Coarse mesh transport

- The method couples Monte Carlo or deterministic response function calculations to deterministic sweeps for converging on coarse mesh interface incident fluxes that are approximated by truncated Legendre polynomials in phase space variables
- Shown to be highly accurate and efficient at the whole core level (3D)
- **Efficiency gain is achieved by shifting almost all of the CPU to precomputation** - a priori Monte Carlo/deterministic calculations in the unique coarse meshes
- Accurate and high fidelity results require high order incident response expansions (Monte Carlo or deterministic transport lattice calculations)
- Leads to a large data library and precomputation time

Coarse mesh transport-2

- Maintaining efficiency and accuracy for large complex (realistic) problems will require
  - optimization of the memory management
  - efficient grid computing in terms of response function management
  - acceleration of Monte Carlo response function calculations (i.e., parallel computing, variance reduction) – no new development needed for the intended application
  - acceleration and optimization of the coarse mesh sweeps
  - memory parallelization/partitioning for high order solutions

Conclusions

- Online or offline high end computing is a must regardless of the method of choice
  - Processing power
  - Memory
  - Disk capacity
- A very important constraint for practical applications is:
  - **The method /code should not require a massive computing power for production and online whole core simulations**

Highlights of Coarse Mesh Transport Method

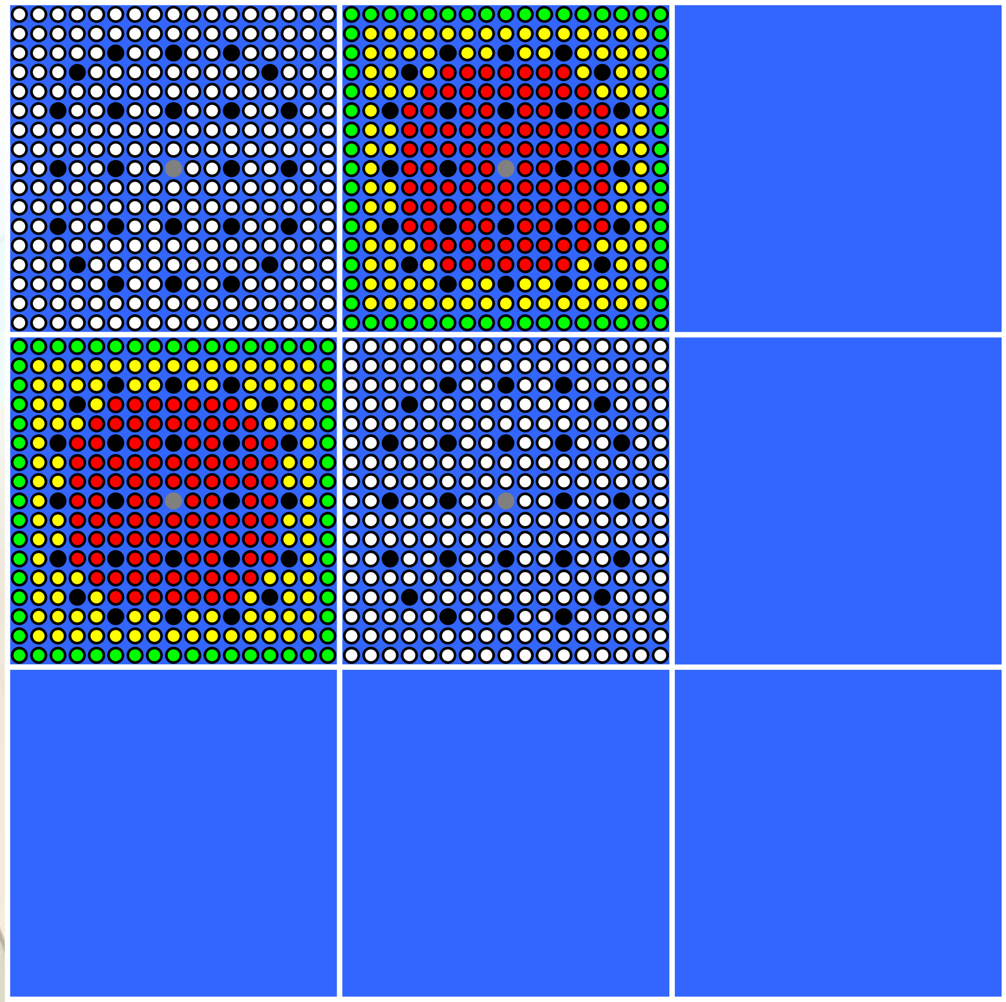
- Coupled neutron/photon transport method
  - Highly efficient making design and online simulation feasible
  - Continuous energy capability has been shown to be possible
  - Complex geometry capability – uses MC to model unique lattices
- Practical for application to current and operating reactors
  - Given the library (precomputed RFs), the code runs very fast on one or few processors
- Similar to the current methods in computing structure
  - Large precomputation time
  - Fast online simulation

Status of COMET

- Currently benchmarking whole core calculation
  - PWR, BWR and CANDU
- Continuous energy photon transport
- Coupled electron and photon transport under development

Coarse Mesh Transport (COMET) Results

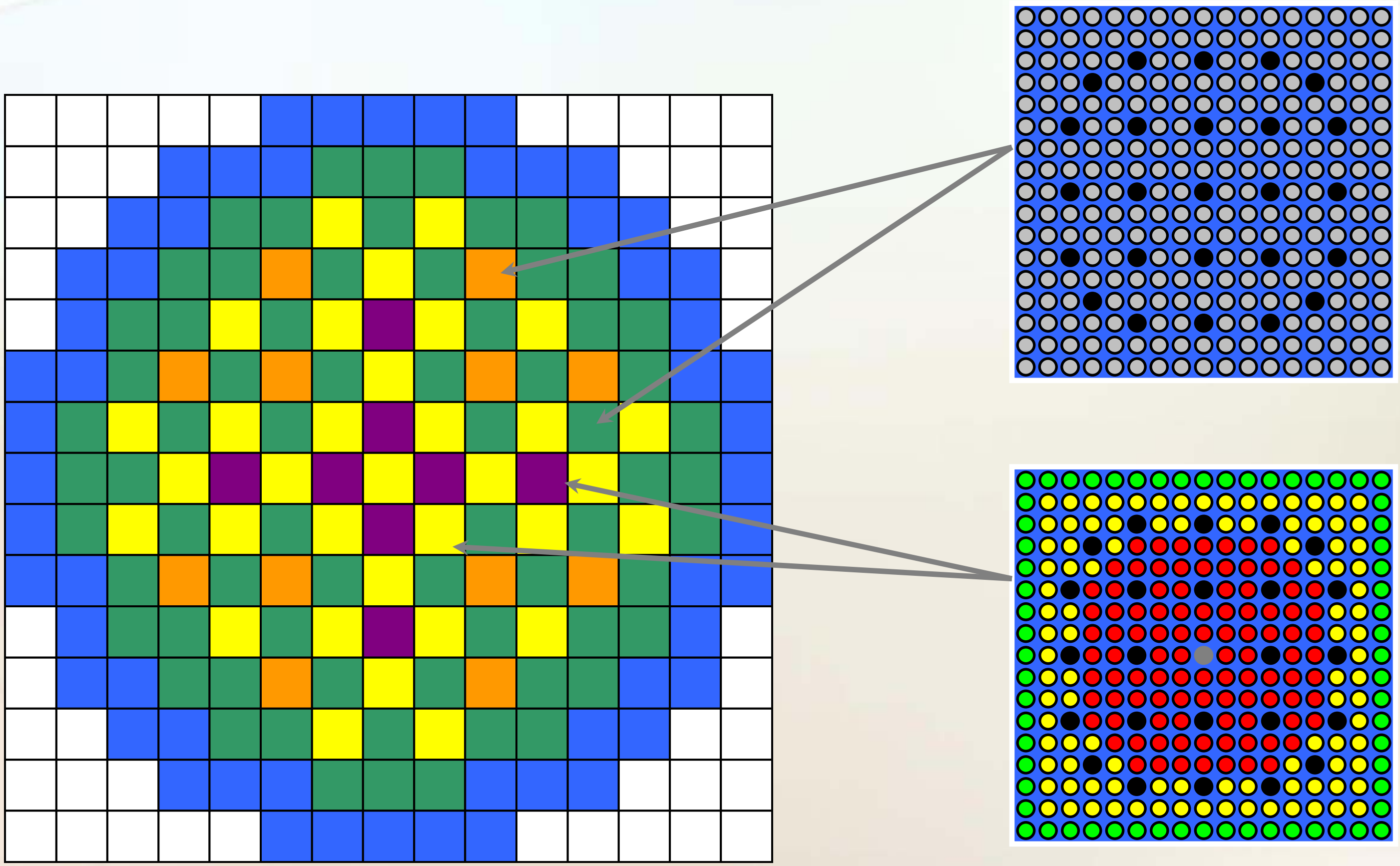
NEA MOX Benchmark Problem



- UO2
- 4.3% MOX
- 7.0% MOX
- 8.7% MOX
- Guide Tube
- Fission Chamber

New Benchmark Problems

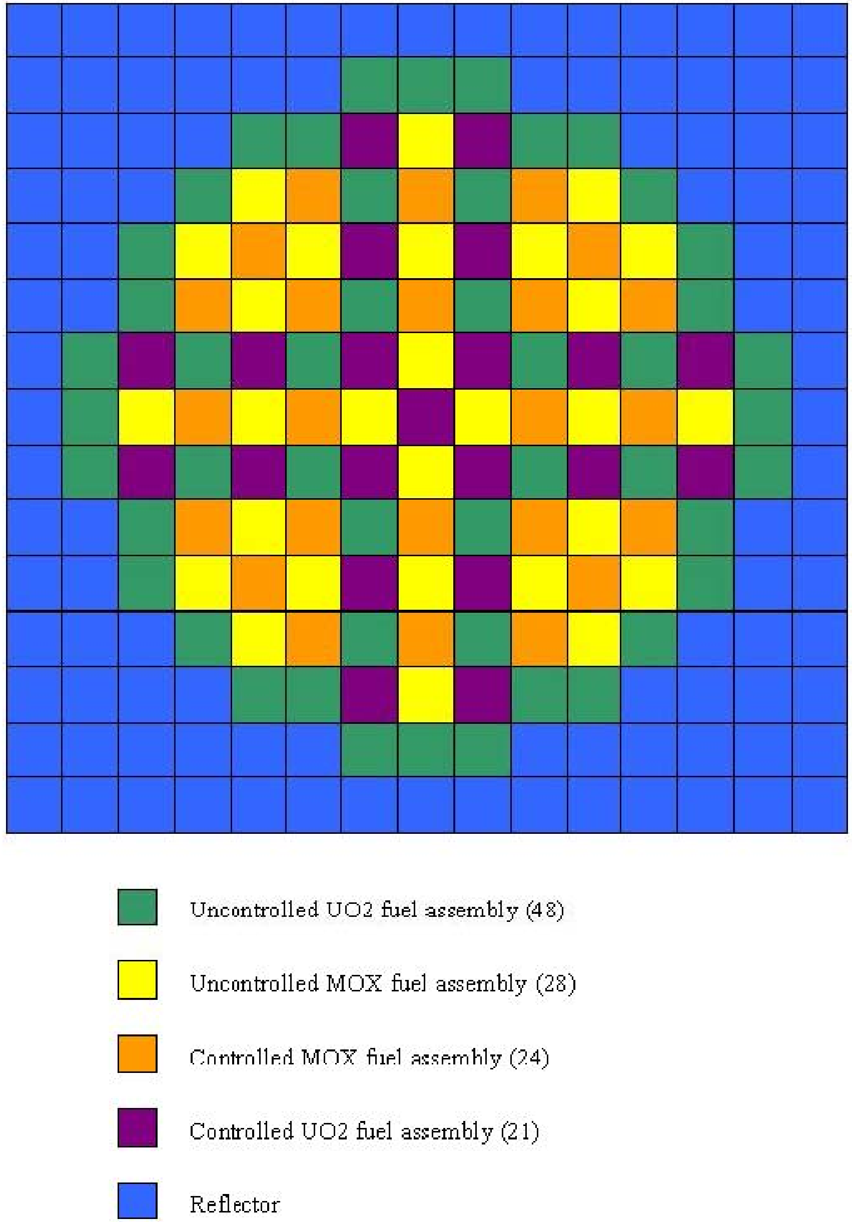
- Full core PWR
  - Extension of NEA MOX Benchmark
  - 225 meshes with 121 fuel assemblies
  - Control Rods in select fuel assemblies



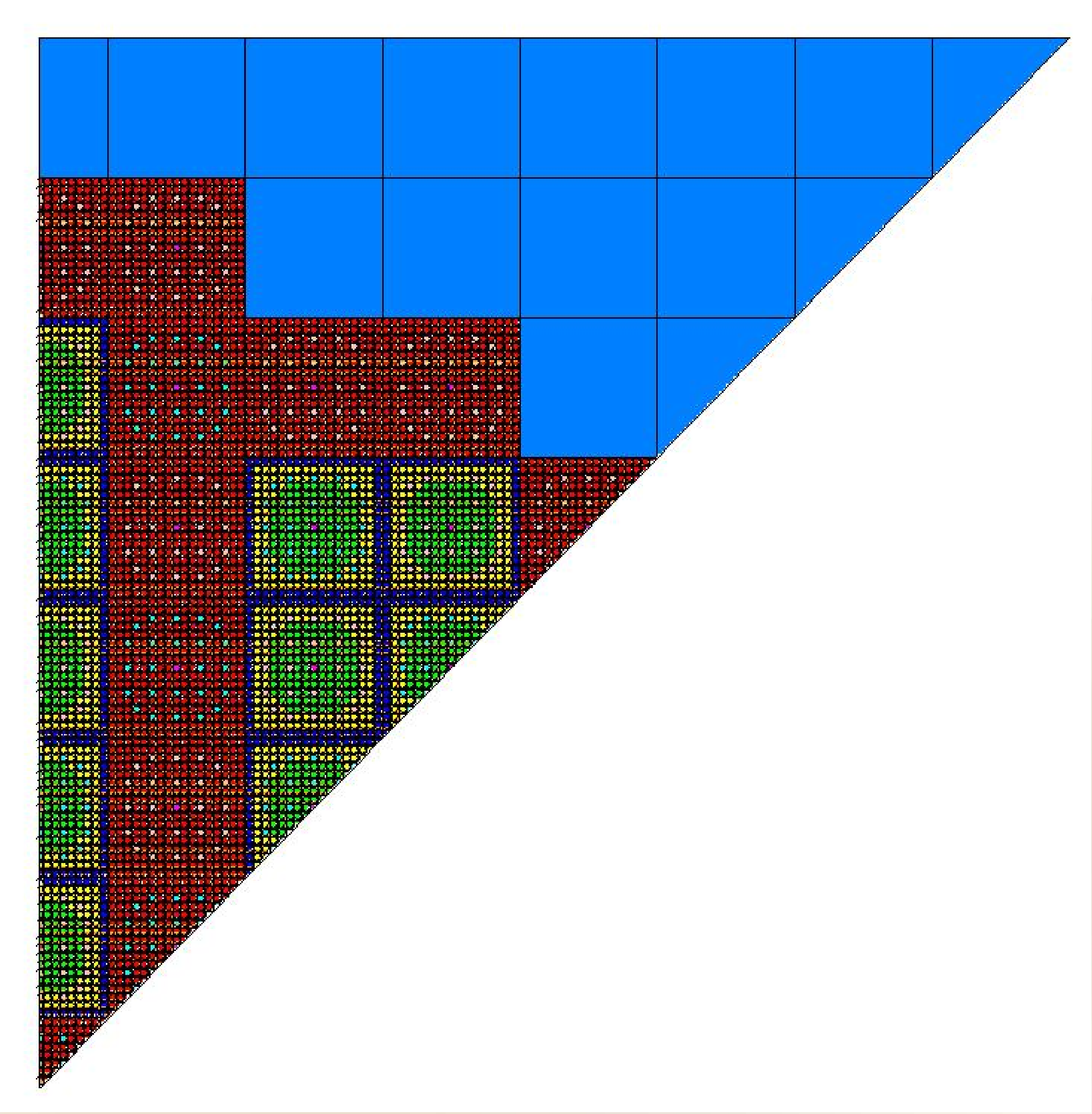
Computational Reactor and Medical Physics Group

Full Core PWR Benchmark Configuration

- 13 x 13 PWR Core
- 121 Fuel Assemblies
  - UO2
    - 48 Uncontrolled Assemblies
    - 21 Controlled Assemblies
  - MOX
    - 28 Uncontrolled Assemblies
    - 24 Controlled Assemblies
- 7 group x.s. from NEA MOX Benchmark


Uncontrolled UO2 fuel assembly (48)
Uncontrolled MOX fuel assembly (28)
Controlled MOX fuel assembly (24)
Controlled UO2 fuel assembly (21)
Reflector

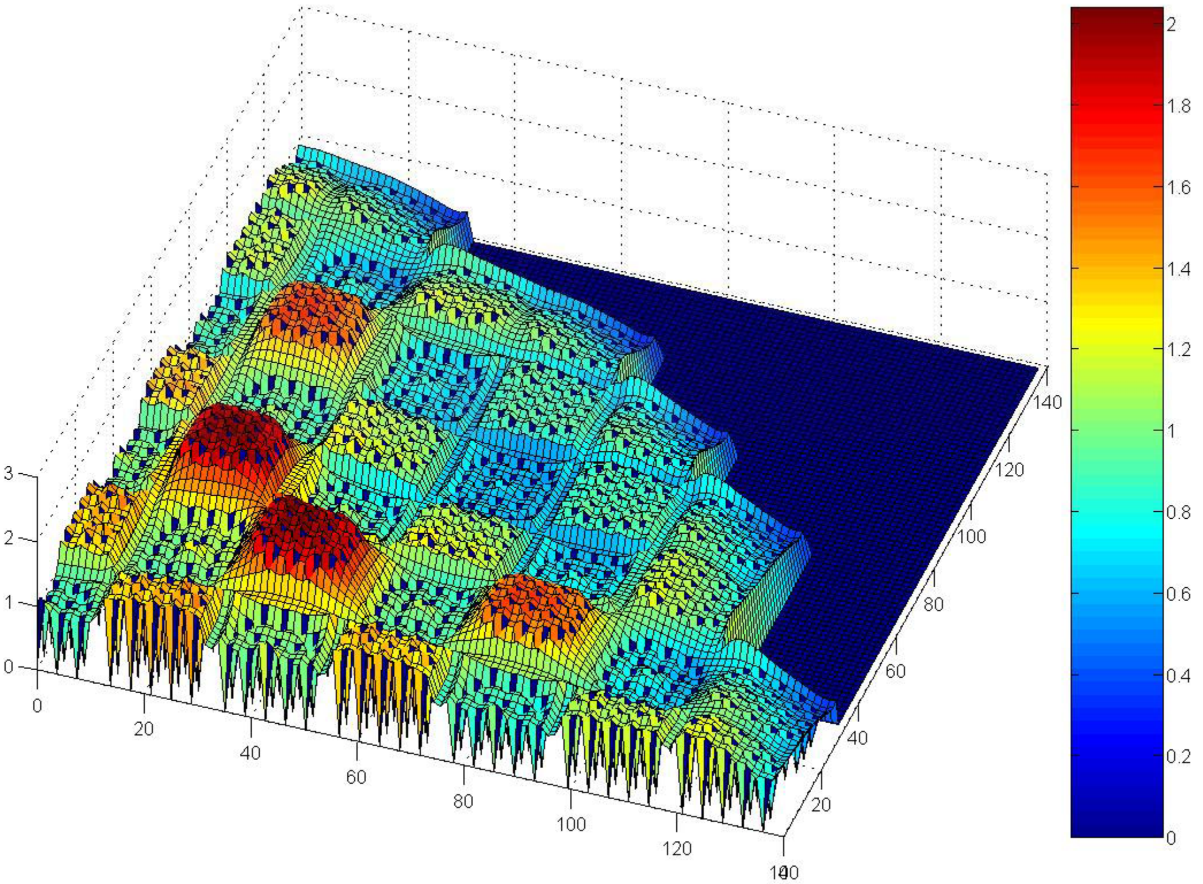
MCNP Reference Model



Reference Solution

- MCNP5 multigroup calculation
- 1/8th of the core
- 1.6 Billion active neutrons
  - 185 hours for active cycles
  - 136 hours for source convergence
- Calculations performed on a 4 node cluster

Reference Solution



Reference pin power distribution expanded to a ¼ core

Reference Solution

- Eigenvalue
  - 1.12623 ± 0.00002
- Pin Power Uncertainty
  - Average Relative Error: 0.11%
  - Maximum Relative Error: 0.23%

Coarse Mesh Solution

- Coarse Mesh Solution performed on Full Core
- Response Functions
  - 1.5 million neutrons
  - Maximum orders {3,2,4}
  - 2 segments per edge
  - 7 groups x.s.
  - k-grid of 1.0, 1.1, 1.2
  - RF Computational Time
  - 20 min/RF for fuel assemblies
    - 2 min/RF for reflector assemblies
    - Entirely Independent Calculations
      - Adding CPU's always gives a linear acceleration

Coarse Mesh Results

	{2,2,2}	{3,2,4}
Eigenvalue RE (%)	-0.02	-0.02
AVG (%)	1.0	0.9
RMS (%)	1.2	1.0
MAX (%)	4.9	3.3
Time (min)	12.8	50.0

- Both Calculations used 0th order acceleration
- Average/Maximum Pin Relative Error
  - {2,2,2} = 0.25/0.34 %
  - {3,2,4} = 0.26/0.35 %
- Convergence Criteria
  - Inner = 10^{-3} , Outer = 10^{-4}

COMET RESULTS (Errors) – 3D NEA MOX (1-Groups)

	{2,2,2,2} (%)	{2,2,2,4} (%)	{3,3,2,4} (%)
RE k	0.10	0.06	0.08
AVG	0.75	0.6	0.6
RMS	0.9	0.8	0.7
MRE	0.7	0.5	0.5
MAX	3.2	2.6	2.7
# RF	81	135	150
CPU Time (s)	107	179	278

3D MOX -2

- RF up to 5th order with 3 million particles for a total of 35 000 response functions
- RF precomputation time – 7 days for the unrodded case on 20 dual core computers
- Average uncertainty of about 0.4%

3D MOX-3

- 7-group, 7 million particles (2nd order RF)
  - ~ 10 days on 20 dual core computers for 2nd order RF (shown below
  - will require 25 days for RFs to reduce max error to 2-3%

	AVG (%)	RMS (%)	MRE (%)	MAX (%)
Errors	1.0	1.5	0.7	9.9
COMET Uncertainty (%)	0.26	-	-	0.49

Questions?